

Nuclear Energy Spectra Calculated from Derived Single-Particle Energies

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Abstract

The usual approach to shell-model calculation is to use experimentally extracted single particle (s.p) energies as a part of an input data to the shell model for nuclear energy calculation. A set of mass-dependent s.p energies for sd-shell calculations derived from realistic forces using a set of two-body correlation with ^{16}O taken as a closed-shell core is used in the present work to determine the energy spectra of nuclei in the upper half of the sd-shell. It is observed that the calculated spectra using the derived s.p energies are in good agreement when compared with those obtained when using experimentally extracted s.p energies. However, both of them showed compression behaviour as compared to the experimental spectra of these nuclei. The results demonstrated that shell-model calculations can be done quite successfully with the s.p energies derived from the interaction.

Keywords: Nuclear Energy Spectra, Single-Particle

1.0 Introduction

For some time now the shell model has come to play a major role in the understanding of nuclear structure, and the use of s.p energies as part of an input data to shell model calculation has received a lot of attention [1, 2, 3]. The combination of this model with the experimental techniques has enabled us to understand the building blocks on which nature is based on at least at the level of protons and neutrons. From this we, of course, make the assumption that the internal degrees of freedom of both protons and neutrons are not excited. Even with the aforesaid assumption, the problem is still a formidable one because this is a many body problem and the dimensions of the Hamiltonian for an A -body system, where $A \geq 3$ is not easily tractable. This means that further assumptions still have to be made. One assumption to be made is to remember that the structure of nuclei with magic numbers such as ^{16}O is particularly stable. One can then assume that in defining the Hamiltonian of an A -system, the part of the Hamiltonian that constitutes the magic core should remain inactive and should contribute a constant energy. We are then left with the model space with which to do our shell model calculations by further assuming that there is no overlap between the core states and the states outside the core, the so-called valence states. The Hamiltonian therefore splits into the core and the valence space [4,5]:

$$\langle H \rangle_{JT} = E_0 + \sum_i e_i + \sum_{i>j,k>l} \langle ij | V_{\text{eff}} | kl \rangle_{JT} \quad (1)$$

where E_0 in this equation is the binding energy of the closed core which is taken to have a constant value.

The middle term, e_i , are the s.p energies, while the last term in equation (1) represents the two-body matrix elements of the residual interaction between the valence orbits i, j, k and l .

Various empirical and theoretical techniques are used in order to determine the two-body matrix elements of the residual interaction [2, 6]. The empirical approach treats all the s.p energies together with the two-

body matrix elements as free parameters. These are adjusted until they fit the experimental spectrum [5]. Several groups have followed this approach with a high degree of success [2, 7]. Yet the microscopic approach demands that these quantities have some theoretical basis. This approach studied by many authors [8, 9], attempts to explain all the experimental properties of nuclei with microscopic theory.

While the energy spectra of various nuclei has been extensively studied in terms of s.p energies extracted from experiment and various two-body matrix elements [10], the spectra of nuclei in terms of the s.p energies derived microscopically has received less attention. Using the method of lowest order constrained variational technique (LOCV) [5], it was shown that the

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shell model calculation can be done quite successfully with s.p energies derived from theory. The LOCV is a very powerful method of calculating both the s.p energies and the two-body matrix elements, very accurately. In Ref [4], the LOCV was used to derive a set of mass-dependent s.p energies for sd-shell model calculations. The aim of this paper is to use the set of s.p energies discussed in Ref. [4] in combination with our two-body matrix elements derived from our two-body effective interaction as well as the Wildenthal's empirically determined two-body matrix elements [2] to calculate the energy spectra of Chlorine, ³⁴Cl nucleus. The rest of the paper is organized as follows: In section 2 we give the summary of the method of how we define our two-body effective interaction for the shell model. In section 3, we give the result of the calculated spectra of ³⁴Cl using the s.p energies given in Ref. [4]. Section 4 is devoted to the summary and conclusion of the paper.

• **The Nuclear Hamiltonian and the Two-Body Effective Interaction for Shell Model Calculation**

In this section we give a summary of the LOCV approach discussed in Refs. [4, 8] for evaluating the two-body effective interactions. The non-relativistic nuclear Hamiltonian for an A-nucleon system is approximated as :

$$H_0 = \sum_i p^2 / 2m + \sum_{i>j} V_N(ij), \quad (2)$$

where $V_N(ij)$ is the nucleon-nucleon (NN) potential and m is the nucleon mass. Since the NN potential of equation (2) is known to have a large repulsive component which makes it difficult to apply the direct Hartree-Fock formula, the Hartree-Fock wave function :

$$\Phi = (A!)^{-1/2} \det \phi_i(\vec{r}_i) \quad (3)$$

must be correlated in the form:

$$\Psi = F\Phi, \quad (4)$$

where the ϕ_i are the s.p basis functions and F is a symmetric product of two-body correlation function [9]

$$F = S \prod_{ij} f_{ij} \quad (5)$$

Such correlations were formulated in order to accommodate the effect of the strong repulsive component of the NN interaction. In this equation, S is the symmetrizer operator. Furthermore, we require that the Hamiltonian be formulated in the rest-frame of the nucleus. This is achieved through a unitary transformation [10]:

$$H_0 \rightarrow \bar{H} = H - p^2 / 2M = \sum_{i>j} (p_{ij}^2 / M + V_N(ij)) \quad (6)$$

Where $M = m_N A$ is the total mass of the nucleus, $p^2 / 2M$ is the translational kinetic energy of the

centre of mass of the nucleus, $\vec{p}_{ij} = 1/\sqrt{2}(\vec{p}_i - \vec{p}_j)$ is the relative momentum of the interacting particles.

For the NN potential, $V_N(ij)$ here after denoted as V_{ij} , we have used the Reid [11] soft-core potential. Owing to the dimensionality problem mentioned above, we chose a model space where only the two-body effective interactions are important, since working with the full shell model Hilbert space is very difficult. The justification for this approach has been fully explained in [10]. The two-body interactions have therefore been formulated in the form (Irvine [10])

$$H_{eff}^{(2)} = \sum_{i>j} (f_2(ij)(p_{ij}^2/M + V_{ij})f_2(ij)) \quad (7)$$

where $f_2(ij)$ are the two-body correlation operators. In previous calculation [8] it was required that the two-body correlation functions should take on the features of the chosen potential used. In the present calculation, we use the Reid [11] soft-core potential which has the form

$$V_{ij} = \sum_k V_{ij}^k \quad (8)$$

where k is a reaction channel which has the central (C), spin-orbit (LS) and tensor (T) components. In a similar manner we have expanded the correlation operators as

$$f_2(ij) = \sum_k f_{ij}^k \quad (9)$$

$$\text{where } f_{ij}^k = f_c^k(r_{ij}) + f_{LS}^k(r_{ij})L.S + f_T^k(r_{ij})S_{ij} \quad (10)$$

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with $f_c^k(r_{ij})$, $f_{LS}^k(r_{ij})$ and $f_T^k(r_{ij})$ representing the correlation functions for the central channel, spin-orbit channel and tensor channel respectively.

Early calculations on nuclear matter and finite nuclei [12] have shown that only central and tensor correlations are more significant. This permits us to parameterize the two-body correlation functions in these channels in the form [13]

$$f_2(ij) = 0, r_{ij} < r_c$$

$$f_2(ij) = \left(1 - e^{-\beta(r_{ij}-r_c)^2}\right) \left(1 + \alpha^k S_{ij}\right), r_{ij} \geq r_c \quad (11)$$

where $r_c = 0.25 \text{ fm}$ and $\beta = 25 \text{ fm}^{-2}$. The parameter α^k represents the strength of the tensor correlation. The two-body matrix elements of the effective Hamiltonian defined in equation (7) were calculated in the harmonic oscillator basis. The general expression for evaluating the two-body matrix elements, is reported in Refs. [4,6]. Furthermore, one can calculate the

single particle energies from the

same interaction according to the equation [4] as:

$$e_i = \sum_{KJT} \frac{(2T+1)(2J+1)}{2(2l+1)} \langle (Kl)JT | H_{eff}^{(2)} | (Kl)JT \rangle_{AS} \quad (12)$$

where in the summation the sum K is limited to the core states and l is the valence space orbital. Note that in

our calculation of equation (12), there are only two free parameters. These are the oscillator size parameter and the strength of the tensor correlations. We vary these to obtain the best set of one- and two-body effective interactions to calculate the ^{34}Cl spectra.

• Results and Discussion

We now use the results of the two-body effective interactions defined in Ref. [4] and the set of s.p energies defined in equation (12) calculated by the method of Ref. [4] for evaluating the energy spectra of Chlorine, ^{34}Cl .

In Fig. 1(a), the calculated spectrum of ^{34}Cl using our interaction is presented together with the experimental spectrum [14, 15] for the positive parity states of ^{34}Cl . For comparison we also present the result of the shell model calculation using the Wildenthal empirical effective interaction [2]. We denote a state by $J_i^\pi; T$ where J is the total angular momentum of the two particle system while T is their corresponding isospin. From Fig.1(a) we see that our calculated energy spectrum is rather compressed when compared with the experimental spectrum. We have repeated the same procedure in Fig. 1(b) but this time with single particle energies extracted from experiment, but this also provides the same result. Indeed, Fiase and Sharma [5], and Hjorth-Jensen *et al* [6] have made a similar observation with regards to forces with a strong tensor component to which the Reid [11] potential used here also belongs. Since our calculated spectra are compressed either with s.p energies calculated from the interaction or with those extracted from experiment, we conclude that our problem resides in our calculated two-body matrix elements. We therefore decided to alter our two-body matrix elements by comparing them with their Wildenthal counterparts. Those matrix elements in our calculation that differed by more than 150 KeV from their Wildenthal counterparts were replaced by Wildenthal values. In doing so we retained only 28 two-body matrix elements from the 63 Pauli allowed two-body matrix elements in our calculation.. The remaining 35 were therefore the Wildenthal empirical matrix elements. We kept the s.p energies fixed at their calculated values. In Fig. 2(a) we noticed an impressive agreement with experiment. The first five experimental levels: 0^+ , 3^+ , 1^+ , 1^+ and 2^+ at energies 0.0, 0.146, 0.461, 0.665 and 1.230 MeV respectively are well reproduced at energies of 0.0, 0.132, 0.278, 0.532 and 1.078 MeV respectively using our s.p energies calculated from the same interaction. When the s.p energies from experiments were used adopting the same procedure, the same states are predicted at energies of 0.0, 0.140, 0.392, 0.601 and 1.192 MeV respectively as shown in Fig. 2(b). For a comparison, we have also calculated the same states using Wildenthal empirical effective interaction. This interaction puts these states at energies 0.0, 0.133, 0.317, 0.661 and 1.143 MeV respectively. Beyond these energies we have no one-to-one correspondence between our calculated spectra and their experimental counterparts. Thus we can claim that our calculated s.p energies are capable of predicting at least the low lying positive parity states of ^{34}Cl .

• Summary and Conclusion

In this paper we have carried out a shell-model study on the energy spectra of ^{34}Cl nucleus. We have found that our two-body effective interactions and the single-particle alone are not capable of providing a good description of the energy spectra of this nucleus. We therefore substituted some of the matrix elements of our effective two-body interaction that differed by more

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than 150 KeV with their counterparts from the Wildenthal empirically fitted interaction and repeated the energy spectra calculation while keeping our s.p energies fixed at their calculated values. With this

procedure, we found that the overall spectra for the low-lying positive parity states for the nucleus in question are in excellent agreement with experiment as well as the result of other workers on this nucleus. Though the calculation of energy spectra such as presented in this paper is not new, it should be noted that in most microscopic shell-model calculations, the set of two-body effective interactions are derived microscopically but the set of s.p energies are extracted from experiment. Our approach here has been to emphasize that the spectra of nuclei can be calculated with s.p energies derived from theory. This should still be regarded as a first-step calculation because we have neither considered the effect of core excited states in our calculation nor have we extended our approach to include the delta resonances in nuclei. We have also not considered electromagnetic properties of this nucleus in our calculations which are a stringent test for a successful shell-model calculation. Yet our model seems to be quite promising in predicting the low-lying energy levels of nuclei.

Fig. 1: Calculated energy spectra of ^{34}Cl nucleus compared with experiment and Wildenthal interaction. (a) is the result of the present calculation with single particle energies derived from the interaction. (b) is the result of the present calculations with single-particle energies extracted from experiment. Notice, that our

interaction gave spectra that is compressed either with single-particle energies from the interaction or those extracted from experiment

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Fig. 2: Calculated energy spectra of ^{34}Cl nucleus compared with experiment and Wildenthal interaction. (a) is the result of the present calculation with single particle energies derived from the interaction. (b) is the result of the present calculations with single-particle energies extracted from experiment.

5.0 References

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